

# Solution of two level system using 3<sup>rd</sup> order Magnus expansion\*

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The solution of a two level system driven by a Laser in the adiabatic limit is determined using third order Magnus expansion. We made the assumption that the laser is on resonance or close to resonance with the Bohr transition. As a consequence of which we are able to obtain a Hamiltonian which commute with itself at different times. We solve the problem using the Sylvester Formula where we make use of the eigenvalues.

## I. INTRODUCTION

The study of the dynamics of two level system has been attracting interest of researchers in different areas ranging from Nuclear magnetic resonance (NMR) [1] to Quantum Computers [2]. The solution of a two level system whose Hamiltonian is closed under Lie algebra can be obtained using Wei-Norman [3] and is pursued by different authors [4, 5]. As application the author in [5], for example, has used the solution obtained via Wei-Norman for quantum computing. The solution obtained via Wei-Norman is exact, yet it is sometimes insightful to get analytical solutions of the dynamics of the system. We here aim to use the knowledge of the eigenvalues to provide analytical solution of two level system using the third order Magnus expansion via Sylvester formula. Moreover the focus in this paper is for an isolate system, however, if we include noise the coherences will be destroyed by the effect of the environment.

The outline of the paper is as follows: in section (II) we introduce the two level system where we describe its Hamiltonian and obtain the equation of motion, in section (III) we use third order Magnus expansion to obtain the solution of the equation of motion, in section (IV) we present the comparison of the solutions of the equation of motion using the third order Magnus expansion and numerical solution. We will also present comparison between first, second and third order Magnus expansions. At last in section (V) we summarize our results and provide an outlook.

## II. THE SYSTEM

The system we consider is shown in fig.(1), we assume to have a two level system with ground state  $|0\rangle$  and excited state  $|1\rangle$ . Suppose the two levels are coupled by a field  $\Omega(t)$  and the laser is off by detuning  $\Delta$ , which is the difference between the laser frequency and the Bohr frequency. We consider an adiabatic population transfer

[6], yet we apply a weak pulse (corresponding to pulse area of  $\pi/2$ ) to avoid transferring all the population, from  $|0\rangle$  to  $|1\rangle$ , as one would have when using pulse area of  $\pi$ . Using  $\pi$  pulse area protocol one could completely transfer the populations from the ground state  $|0\rangle$  to the excited state  $|1\rangle$  [7].

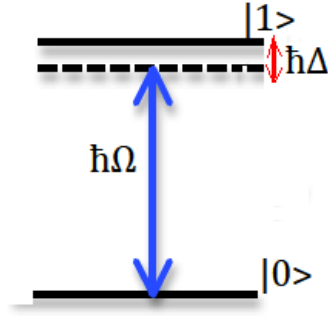


FIG. 1. (Color online) Two level system. Detuning  $\hbar\Delta$  and coupling  $\hbar\Omega(t)$

The Hamiltonian under Rotating Wave Approximation (RWA) and in the interaction picture is known to be [6, 8].

$$\hat{H}(t) = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega(t) \\ \Omega(t) & 2\Delta \end{pmatrix} \quad (1)$$

We use the Pauli matrices as our generators, and they are given by [2]

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2)$$

In terms of which we expand the density matrix as well as the Hamiltonian [9].

$$\hat{\rho}(t) = \frac{\hat{I}}{2} + \frac{1}{2} \sum_{j=1}^3 S_j(t) \hat{\sigma}_j$$

$$\hat{H}(t) = \frac{\hbar}{2} \left[ \left( \sum_k^2 \omega_k \right) \hat{I} + \sum_{j=1}^3 \gamma_j(t) \hat{\sigma}_j \right] \quad (3)$$

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where  $\hbar\omega_k$  is energy of level  $k$  and  $\hat{I}$  is the identity operator. The coefficients  $S_j(t)$  and  $\gamma_j(t)$  are given by [9]

$$S_j(t) = \text{Tr}(\hat{\rho}(t)\hat{\sigma}_j) \quad (4a)$$

$$\hbar\gamma_j(t) = \text{Tr}(\hat{H}(t)\hat{\sigma}_j) \quad (4b)$$

the generators  $\hat{\sigma}_j$  are the Pauli matrices and has the following properties [9]

$$\begin{aligned} \text{Tr}(\hat{\sigma}_i\hat{\sigma}_j) &= 2\delta_{ij} \\ [\hat{\sigma}_i, \hat{\sigma}_j] &= 2i\epsilon_{ijk}\hat{\sigma}_k \end{aligned} \quad (5)$$

Based on this, and following the same procedure as in [9, 10] we get the equation of motion for the coherence vector. If we now form vector  $\vec{S} = (S_1(t), S_2(t), S_3(t))^T$  whose elements are the expectation value of the Pauli matrices as given by Eq.(4a), we readily obtain the equation of motion to be

$$\frac{d}{dt}\vec{S} = g\vec{S} \quad (6)$$

where  $g$  is given by

$$g = \begin{pmatrix} 0 & \Delta & 0 \\ -\Delta & 0 & -\Omega(t) \\ 0 & \Omega(t) & 0 \end{pmatrix} \quad (7)$$

Although one can solve this equation of motion numerically, we are here interested in finding a comparison between numerical and analytical solution. We will solve Eq.(6) both numerically and analytically, we then compare the two solutions for different values of detuning.

### III. MAGNUS APPROXIMATIONS

One way of solving equation Eq.(6) is given by the Magnus Approximation [11]. The Magnus expansion, named after Wilhem Magnus, provides an exponential representation of the solution of a first order linear homogenous equation for linear operator. Given an  $N \times N$  coefficient matrix  $g(t)$  we wanted to solve the initial value problem associated with the linear ordinary differential equation, which in our case is the equation of motion for the coherence vectors given by, along with its initial condition:

$$\frac{d\vec{S}(t)}{dt} = g(t)\vec{S}(t) \quad \vec{S}(0) = S_0 \quad (8)$$

We now make the assumption that the laser is on resonance or close to resonance, meaning  $\Delta = 0$  or is negligibly small and consequently the matrix  $g$  now commutes with itself at different times, that is  $[g(t_1), g(t_2)] = 0$ . The approach proposed by Magnus to solve the matrix initial value problem is to express the solution of the exponential of a certain  $N \times N$  function  $G(t, t_0)$

$$\vec{S}(t) = e^{G(t,0)}\vec{S}(0) \quad (9)$$

which is subsequently written as a series expansion

$$G(t, 0) = \sum_{k=1}^{\infty} G_k(t, 0) \quad (10)$$

writing  $G(t, 0) = G(t)$  for simplicity, the first three series reads thus

$$\begin{aligned} G_1(t) &= \int_0^t g(t_1) dt_1 \\ G_2(t) &= \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} [g(t_1), g(t_2)] dt_2 \\ G_3(t) &= \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} [g(t_1), [g(t_2), g(t_3)]] dt_3 \\ &\quad + \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} [g(t_3), [g(t_2), g(t_1)]] dt_3 \end{aligned} \quad (11)$$

where  $[g_1, g_2] = g_1g_2 - g_2g_1$ . In search of better approximation one needs to include more terms in the Magnus expansion. In this paper we will be considering only the first three series  $G_k(t)$ ,  $k = 1, 2, 3$ , therefore the solution for Eq.(6) now becomes

$$\vec{S}(t) = e^{G^{(3)}(t)}\vec{S}(0) \quad (12)$$

where  $G^{(3)}(t)$  is sum of the three series given in Eq.(11). One way of determining  $e^{G^{(3)}}$  is using the Sylvester formula. The Sylvester formula is a way of solving any exponential function by making use of eigenvalues [12, 13]. To this end let  $\gamma_j$  be an eigenvalue of  $G^{(3)}(t)$ , we thus can write the exponent using Sylvester formula (iff we have distinct eigenvalues) as

$$e^{G^{(3)}(t)} = \sum_{j=1}^3 e^{\gamma_j} \prod_{j \neq k=1}^3 \frac{G^{(3)}(t) - \gamma_j I}{\gamma_k - \gamma_j} \quad (13)$$

The third order Magnus is obtained to be of the form

$$G^{(3)}(t) = \begin{pmatrix} 0 & \eta(t) & \lambda(t) \\ -\eta(t) & 0 & -\zeta(t) \\ -\lambda(t) & \zeta(t) & 0 \end{pmatrix} \quad (14)$$

where  $\eta(t) = \Delta'(t) + \lambda_1(t)$  and  $\zeta(t) = \Omega'(t) + \lambda_2(t)$  with  $\Omega'(t) = \int_0^t \Omega(t_1) dt_1$ ,  $\Delta'(t) = \int_0^t \Delta dt_1$  and

$$\begin{aligned} \lambda(t) &= \frac{\Delta}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 (\Omega_1 - \Omega_2) \\ \lambda_1(t) &= -\frac{\Delta}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 (\Omega_1(\Omega_2 - 2\Omega_3) + \Omega_2\Omega_3) \\ \lambda_2(t) &= -\frac{\Delta^2}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 (\Omega_1 - 2\Omega_2 + \Omega_3) \end{aligned} \quad (15)$$

where we used the notation  $\Omega_j = \Omega(t_j)$  for simplicity. In what follows we omit the time argument  $(t)$  unless it is needed for clarity. The eigenvalues of  $G^{(3)}$ , are readily

obtained to be  $\{0, -i\xi, i\xi\}$ , where  $\xi = \sqrt{\lambda^2 + \zeta^2 + \eta^2}$ . It is worth pointing out here that we have distinct eigenvalues. Therefore we can now express our solution for the coherence vector in terms of the Sylvester formula. To this end, making use of the eigenvalues and Eq.(12) along with Eq.(13) and noting that the system is initially prepared to be on the ground state, we find the following solution

$$\vec{S}(t) = \begin{pmatrix} \frac{-\zeta\eta - \zeta\eta \cos \xi - \lambda\xi \sin \xi}{\xi^2} \\ \frac{-\lambda\eta + \lambda\eta \cos \xi - \zeta\xi \sin \xi}{\xi^2} \\ \frac{\eta^2 + (\lambda^2 + \zeta^2) \cos \xi}{\xi^2} \end{pmatrix} \quad (16)$$

If however we consider only the first term in the Magnus expansion, it follows that  $\lambda = \lambda_1 = \lambda_2 = 0$ , and accordingly we have to modify our solution– Eq.(16) to be

$$\vec{S}(t) = \begin{pmatrix} \frac{\Delta'\Omega'}{\xi^2} (-1 + \cos \xi) \\ -\frac{\Omega'}{\xi} \sin \xi \\ \frac{\Delta'^2}{\xi^2} + \frac{\Omega'^2}{\xi^2} \cos \xi \end{pmatrix} \quad (17)$$

where now  $\xi = \sqrt{\Delta'^2 + \Omega'^2}$

#### IV. RESULTS AND DISCUSSION

It is worth pointing out here that because of the pulse area we used, i.e.  $\frac{\pi}{2}$  we do not see the Rabi oscillations, we instead see that, at the end of the pulse interaction, we are able to create superpositions between states  $|0\rangle$  and  $|1\rangle$ . To see the Rabi oscillation, where in the population fluctuates between states  $|0\rangle$  and  $|1\rangle$ , one needs to use a laser whose pulse area is an integral multiple of  $\pi$ . For exact resonance where  $\Delta = 0$ , as can be seen in Fig.(2), the solutions obtained using Magnus expansion and numerical solution are identical. This is because all the commutator terms are dependent on  $\Delta$ . But if we have a non-zero detuning but small value the results obtained numerically and using Magnus expansion may differ. We see in Fig.(3a) comparison of solutions obtained via numerical and first order Magnus. As we took a very small value of detuning we have a very small value resulted from the commutation of the Hamiltonian with itself at different times. Consequently the solution we obtained using the first order Magnus approximation is close to the numerical but does not fully agree with the numerical solution. Whereas if we use the third order Magnus expansion as it means we include more correction terms the the solution is seen to be improved Fig.(3b)

#### V. CONCLUSION

In conclusion we have shown in this paper that for a two level system which is either on resonance or close to

resonance one can obtain an analytical solution of the

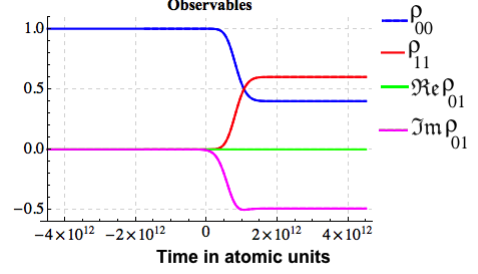


FIG. 2. (Color online) Solution using first order Magnus, i.e. when  $\lambda = \lambda_1 = \lambda_2 = 0$  and  $\Delta = 0$ . The solid lines are numerical solution whereas the dashed lines are analytical solution. Key: blue= $\rho_{00}$ , red= $\rho_{11}$ , green=Real part of  $\rho_{01}$ , and magenta=Imaginary part of  $\rho_{01}$

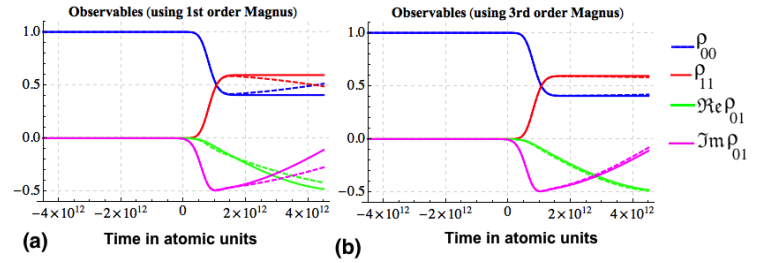


FIG. 3. (Color online) Solution using (a) first order Magnus, i.e. when  $\lambda = \lambda_1 = \lambda_2 = 0$  (b) third order Magnus, i.e. when  $\lambda = \lambda_1 = \lambda_2 \neq 0$ . The solid lines are numerical solution whereas the dashed lines are analytical solution. Key: blue= $\rho_{00}$ , red= $\rho_{11}$ , green=Real part of  $\rho_{01}$ , and magenta=Imaginary part of  $\rho_{01}$

dynamics which is very much close to the exact solution obtained via numerical. If the system is far from resonance case we recommend to include more of the commutation terms of the exponent to obtain a better approximate of the solution. To reiterate, for exact resonance where  $\Delta = 0$  the solutions obtained using Magnus expansion and numerical solution are identical. This is because all the commutator terms are dependent on  $\Delta$ . But if we have a non-zero detuning but small value the results obtained numerically and using  $3^{rd}$  order Magnus expansion agrees quite well. If however the value of the detuning is big then the solutions differ. We plan to extend the approach for three-level system in the  $SU(3)$  dynamics. One point worth mentioning is that the system we have considered is closed system but if we include a noise the coherence would be affected negatively.

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